

Self-Consistent Nuclear Shell-Model Calculation Starting from a Realistic NN Potential

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First self-consistent realistic shell-model calculation for the light p -shell nuclei is performed, starting from the high-precision nucleon-nucleon (NN) CD-Bonn potential. This realistic potential is renormalized deriving a low-momentum NN potential $V_{\text{low-k}}$ that preserves exactly the two-nucleon low-energy physics. This $V_{\text{low-k}}$ is suitable to derive a self-consistent Hartree-Fock basis that is employed to derive both effective single-particle energies and residual two-body matrix elements for the shell-model hamiltonian. Results obtained show the reliability of such a fundamental microscopic approach.

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The nuclear shell model is the foundation upon which the understanding of the main features of the structure of the atomic nucleus is based. In such a frame, a central role is performed by the auxiliary one-body potential U , which has to be introduced in order to break up the nuclear hamiltonian as the sum of a one-body component H_0 , which describes the independent motion of the nucleons, and a residual interaction H_1 :

$$H = \sum_{i=1}^A \frac{p_i^2}{2m} + \sum_{i<j} V_{ij} = T+V = (T+U)+(V-U) = H_0+H_1 \quad (1)$$

Once H_0 has been introduced, it is possible to define a reduced Hilbert space, the model space, in terms of a finite subset of H_0 's eigenvectors. In this way the unfeasible task of diagonalizing the many-body hamiltonian (1) in a infinite Hilbert space, may be reduced to the one of solving an eigenvalue problem for an effective hamiltonian in a finite model space.

During the last forty years, a lot of efforts have been devoted to derive effective shell-model hamiltonians, starting from free nucleon-nucleon (NN) potentials V_{NN} , which reproduce with extreme accuracy the NN scattering data and the deuteron properties (see for instance [1]). In particular, during the last ten years many realistic shell-model calculations have been performed to describe quantitatively with a great success the properties of nuclei over a wide mass range [2, 3, 4, 5, 6].

In all these studies, for the sake of simplicity, a harmonic oscillator potential has been adopted as auxiliary potential. This choice simplifies the computation of the two-body interaction matrix elements, as well as the derivation of the effective hamiltonian, by way of a degenerate time-dependent perturbation theory [7, 8].

A more fundamental microscopic choice for U is the Hartree-Fock (HF) potential, that is self-consistently derived from the free potential V_{NN} . Such a choice leads to a so-called self-consistent shell model [9]. It

is well known, however, that modern realistic NN potentials cannot be used directly to calculate a HF self-consistent potential, owing to their strong repulsion at short distances. A traditional approach to this problem is the Brueckner-Hartree-Fock (BHF) procedure, where the self-consistent potential is defined in terms of the reaction matrix vertices G [10]. However, this approach cannot be considered the basis for a fully self-consistent realistic shell-model calculation [9], because the choice of the BHF potential for states above the Fermi surface cannot be uniquely defined [11].

Recently, a new technique to renormalize the short-range behavior of a realistic NN potential by integrating out its high-momentum components has been introduced [12]. The resulting low-momentum potential $V_{\text{low-k}}$ is a smooth potential that preserves the low-energy physics of V_{NN} and can be used directly to derive a self-consistent HF potential [13]. This paves the way to perform a full self-consistent realistic shell-model calculation.

In this Letter, we present results of such a kind of shell-model calculation for light p -shell nuclei, starting from the high precision CD-Bonn NN potential [14].

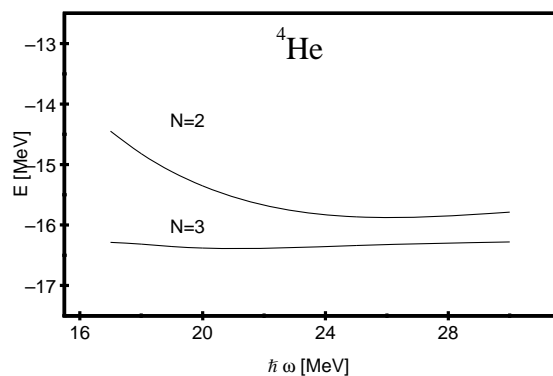


FIG. 1: Behavior of E_{HF} with $\hbar\omega$ and N for ${}^4\text{He}$.

First, for the sake of clarity, we outline the path through which our calculation winds up. The first step

consists in deriving from the CD-Bonn potential a low-momentum potential $V_{\text{low-k}}$ defined within a cutoff momentum Λ . This is done in the spirit of the renormalization group theory so obtaining a smooth potential which preserves exactly the on-shell properties of the original V_{NN} [12]. In Ref. [12] a detailed discussion has been done about the value of Λ and a criterion for its choice. According to this criterion, we have used here $\Lambda = 2.1 \text{ fm}^{-1}$. The so obtained $V_{\text{low-k}}$, hermitized using the procedure based on Choleski decomposition suggested in Ref. [15], has been used directly to solve the HF equations for ${}^4\text{He}$ doubly closed-shell core. We remove the spurious center-of-mass kinetic energy [16] writing the kinetic energy operator T as

$$T = \frac{1}{2Am} \sum_{i < j} (\mathbf{p}_i - \mathbf{p}_j)^2 . \quad (2)$$

So, the hamiltonian can be re-written as

$$H = \left(1 - \frac{1}{A}\right) \sum_{i=1}^A \frac{p_i^2}{2m} + \sum_{i < j} \left(V_{ij} - \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{mA}\right) . \quad (3)$$

The details of our HF procedure may be found in Ref. [13]. In our calculations the HF single-particle (SP) states are expanded in a finite series of $N = 3$ harmonic-oscillator wave-functions for ${}^4\text{He}$. This truncation is sufficient to ensure that the HF results do not significantly depend on the variation of the oscillator constant $\hbar\omega$, as shown in Fig. 1, where the behavior of the HF ground-state energy versus $\hbar\omega$ has been reported for different values of N . The value of $\hbar\omega$ adopted here is 18 MeV, as derived from the expression $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$ [17].

TABLE I: Experimental [22] and theoretical SP energies (referred to ${}^4\text{He}$ closed-shell core) calculated including up to second- and third-order diagrams in $V_{\text{low-k}}$. The experimental widths of the states are also given. Energies are in MeV.

	2nd order	3rd order	Expt.	Γ
$\pi 0p_{3/2}$	1.109	1.355	1.97	1.23
$\pi 0p_{1/2}$	4.800	4.970	3.46	6.60
$\nu 0p_{3/2}$	-0.081	0.202	0.89	0.65
$\nu 0p_{1/2}$	3.796	3.984	2.16	5.57

The HF SP eigenvectors define the basis to be used for our shell-model calculation. More precisely, we assume that doubly-magic ${}^4\text{He}$ is an inert core and let the valence nucleons occupy the two HF orbits $0p_{3/2}$ and $0p_{1/2}$.

The next step is to derive the effective hamiltonian for the chosen model space. Starting from the time-dependent perturbation theory [7], the effective hamil-

tonian is written in operator form as

$$H_{\text{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} + \dots , \quad (4)$$

where \hat{Q} is the irreducible vertex function \hat{Q} -box composed of irreducible valence-linked diagrams, and the integral sign represents a generalized folding operation. \hat{Q}' is obtained from \hat{Q} by removing terms of first order in $V_{\text{low-k}}$.

TABLE II: Experimental and calculated energy levels, in MeV, in ${}^6\text{Li}$ and ${}^6\text{He}$. The calculated results obtained including diagrams up to second and third order in $V_{\text{low-k}}$ are compared. See text for comments.

${}^6\text{Li}$	Expt.	3rd order	2nd order
Binding energy	31.995	31.501	32.198
$E_x(1_1^+0)$	0.0	0.0	0.0
$E_x(3^+0)$	2.186	1.912	1.757
$E_x(0^+1)$	3.563	2.627	2.401
$E_x(2^+0)$	4.312	5.215	5.170
$E_x(2_1^+1)$	5.366	4.911	4.590
$E_x(1_2^+0)$	5.65	7.825	7.305

${}^6\text{He}$	Expt.	3rd order	2nd order
Binding energy	29.269	29.797	30.837
$E_x(0_1^+1)$	0.0	0.0	0.0
$E_x(2^+1)$	1.8	2.108	2.072

We take the \hat{Q} -box to be composed of one- and two-body diagrams through third order in $V_{\text{low-k}}$.

After the \hat{Q} -box is calculated, the energy-independent H_{eff} is then obtained by summing up the folded-diagram series of Eq. (4) to all orders using the Lee-Suzuki iteration method [8]. However, such a method is appropriate for degenerate model spaces only, this is the case when using a harmonic oscillator basis, as pointed out before.

The model space we are dealing with is non-degenerate, the unperturbed HF SP energies (respect to ${}^4\text{He}$ closed-shell core) being 4.217 and 7.500 MeV for $\pi 0p_{3/2}$ and $\pi 0p_{1/2}$, 3.106 and 6.577 MeV for $\nu 0p_{3/2}$ and $\nu 0p_{1/2}$, respectively. So we use a generalization of the Lee-Suzuki iteration method to sum up the folded diagram series, expressed, in the case of non-degenerate model spaces, in terms of the multi-energy \hat{Q} -boxes [18]. To our knowledge this is the first time that the above technique has been employed to derive a realistic shell-model effective interaction.

As mentioned before, H_{eff} contains one-body contributions, the sum of all these contributions (the so-called \hat{S} -box [19]) is what actually determines the SP energies that should be used in a shell-model calculation. It is customary, however, to use a subtraction procedure [19] so that only the two body terms of H_{eff} are retained and

TABLE III: Experimental and calculated energies (MeV) and electromagnetic properties in ${}^7\text{Li}$. The reduced transition probabilities are expressed in W.u..

${}^7\text{Li}$	Expt.	Calc.
Binding energy	39.243	39.556
$E_x(\frac{3}{2}^-\frac{1}{2})$	0.0	0.0
$E_x(\frac{1}{2}^-\frac{1}{2})$	0.478	0.498
$E_x(\frac{7}{2}^-\frac{1}{2})$	4.652	3.998
$E_x(\frac{5}{2}^-\frac{1}{2})$	6.604	5.993
$E_x(\frac{5}{2}^-\frac{1}{2})$	7.454	7.213
$E_x(\frac{3}{2}^-\frac{1}{2})$	8.75	8.985
$E_x(\frac{1}{2}^-\frac{1}{2})$	9.09	9.899
$E_x(\frac{7}{2}^-\frac{1}{2})$	9.57	9.564
$E_x(\frac{3}{2}^-\frac{3}{2})$	11.24	9.206
Q_{gs} [e mb]	-40.6(8)	-24.4
μ_{gs} [nm]	+3.256	+4.28
$B(E2; \frac{1}{2}^-\frac{1}{2} \rightarrow \frac{3}{2}^-\frac{1}{2})$	19.7(1.2)	9.71
$B(E2; \frac{7}{2}^-\frac{1}{2} \rightarrow \frac{3}{2}^-\frac{1}{2})$	4.2	4.18
$B(M1; \frac{1}{2}^-\frac{1}{2} \rightarrow \frac{3}{2}^-\frac{1}{2})$	2.75(14)	2.37

the SP energies are taken from the experimental data regarding the low lying spectra of the nuclei with one neutron or proton outside the inert core. In this calculation we have followed a more fundamental approach, where the SP energies are the theoretical ones obtained from the \hat{S} -box calculation (see Table I).

TABLE IV: Experimental and calculated electromagnetic properties in ${}^6\text{Li}$. The reduced transition probabilities are expressed in W.u..

${}^6\text{Li}$	Expt.	Calc.
Q_{gs} [e mb]	-0.818(17)	-0.442
μ_{gs} [nm]	+0.822	+0.866
$B(E2; 3_1^+0 \rightarrow 1^+0)$	16.5(1.3)	6.61
$B(E2; 2^+0 \rightarrow 1_1^+0)$	6.8(3.5)	6.45
$B(M1; 0^+1 \rightarrow 1_1^+0)$	8.62(18)	9.01
$B(M1; 2_1^+1 \rightarrow 1_1^+0)$	0.083(15)	0.154

In Tables II-VIII we compare experimental binding energies, low-energy spectra, and electromagnetic properties of ${}^6\text{Li}$, ${}^6\text{He}$, ${}^7\text{Li}$, ${}^7\text{Be}$, ${}^8\text{Be}$, ${}^8\text{Li}$, and ${}^8\text{B}$ [20, 21, 22] with calculated ones. All calculations have been performed using the OXBASH shell-model code [23]. A quantitative amount of data for different nuclei is taken into account in order to verify the reliability of a self-consistent shell-model calculation. As regards binding energy results, it is well known that shell-model calculations give ground state energies referred to the closed-shell core. In our approach, we can consistently calculate the ${}^4\text{He}$ binding energy by means of the Goldstone linked-cluster expansion [13]. So, our theoretical

TABLE V: Same as Table IV, but for ${}^7\text{Be}$.

${}^7\text{Be}$	Expt.	Calc.
Binding energy	37.600	37.751
$E_x(\frac{3}{2}^-\frac{1}{2})$	0.0	0.0
$E_x(\frac{1}{2}^-\frac{1}{2})$	0.429	0.469
$E_x(\frac{7}{2}^-\frac{1}{2})$	4.57(5)	3.922
$E_x(\frac{5}{2}^-\frac{1}{2})$	6.73(10)	5.782
$E_x(\frac{5}{2}^-\frac{1}{2})$	7.21(6)	7.123
μ_{gs} [nm]	-1.398(15)	-1.013
$B(M1; \frac{1}{2}^-\frac{1}{2} \rightarrow \frac{3}{2}^-\frac{1}{2})$	2.07(27)	1.81

binding energies are obtained summing the ground state energies of the open-shell nuclei to the calculated ${}^4\text{He}$ binding energy, whose value is 25.967 MeV including up to third-order contributions. Electromagnetic properties have been calculated using effective operators [24] which take into account core-polarization effects.

TABLE VI: Experimental and calculated energies (MeV) in ${}^8\text{Be}$.

${}^8\text{Be}$	Expt.	Calc.
Binding energy	56.50	54.010
$E_x(0_1^+0)$	0.0	0.0
$E_x(2_1^+0)$	3.04	2.985
$E_x(4_1^+0)$	11.40	10.056
$E_x(2_1^+1)$	16.63	15.889
$E_x(2_2^+0)$	16.92	15.174
$E_x(1_1^+1)$	17.64	15.927
$E_x(1_1^+0)$	18.15	15.070
$E_x(3_1^+1)$	19.01	18.863
$E_x(3_1^+0)$	19.24	16.983
$E_x(4_2^+0)$	19.86	21.191

TABLE VII: Same as Table IV, but for ${}^8\text{Li}$.

${}^8\text{Li}$	Expt.	Calc.
Binding energy	41.276	44.365
$E_x(2_1^+1)$	0.0	0.0
$E_x(1_1^+1)$	0.981	0.922
$E_x(3_1^+1)$	2.255	2.074
$E_x(1_2^+1)$	3.21	4.667
$E_x(4_1^+1)$	6.53	6.929
$E_x(0_1^+2)$	10.822	8.230
Q_{gs} [e mb]	24(2)	26.7
μ_{gs} [nm]	+1.653	+2.89
$B(M1; 1_1^+1 \rightarrow 2_1^+1)$	2.8(9)	2.67
$B(M1; 3_1^+1 \rightarrow 2_1^+1)$	0.29(13)	0.38

In Table II we compare calculated binding energies and

spectra of ${}^6\text{Li}$ and ${}^6\text{He}$, obtained including contributions up to second- and third-order in perturbation theory. In all other tables calculated quantities refer to a third-order H_{eff} .

From the inspection of Tables II-VIII, we can conclude that the overall agreement between theory and experiment may be considered to be quite satisfactory. This agreement is of the same quality, and in some cases even better, of that obtained in our previous work [25], where a realistic shell-model calculation for p -shell nuclei was carried out within the framework of the semi-phenomenological two-frequency shell model. It is worth to note that the inclusion of a realistic three-body force could lead to an overall improvement in the agreement with experiment, as shown in Refs. [26, 27]

TABLE VIII: Experimental and calculated energies (MeV) and electromagnetic properties in ${}^8\text{B}$.

${}^8\text{B}$	Expt.	Calc.
Binding energy	37.74	40.429
$E_x(2_1^+ 1)$	0.0	0.0
$E_x(3_1^+ 1)$	2.32	2.061
$E_x(0_1^+ 2)$	10.619	8.245
$Q_{\text{gs}} [e \text{ mb}]$	64.6(1.5)	40.1
$\mu_{\text{gs}} [\text{nm}]$	+1.036	+1.73

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